Universal Markovian reduction of Brownian particle dynamics

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Non-Markovian processes can often be turned Markovian by enlarging the set of variables. Here we show, by an explicit construction, how this can be done for the dynamics of a Brownian particle obeying the generalized Langevin equation. Given an arbitrary bath spectral density J_0, we introduce an orthogonal transformation of the bath variables into effective modes, leading stepwise to a semi-infinite chain with nearest-neighbor interactions. The transformation is uniquely determined by J_0 and defines a sequence $\{J_n\}_{n\in\mathbb{N}}$ of residual spectral densities describing the interaction of the terminal chain mode, at each step, with the remaining bath. We derive a simple, one-term recurrence relation for this sequence, and show that its limit is the quasi-Ohmic expression provided by the Rubin model of dissipation. Numerical calculations show that, irrespective of the details of J_0, convergence is fast enough to be useful in practice for an effective Markovian reduction of quantum dissipative dynamics.

Introduction. As is well known, the study of open systems, in both the classical and quantum case, is a subject of major interest in physics, chemistry, and various other disciplines. In many applications and fundamental experiments, one is faced with the reduced dynamics of a relatively simple subsystem which can be manipulated and measured, while the environment is only partially under control. A thorough understanding of the ensuing dynamics has been obtained for the Markovian case, in which feedback from the environment to the system can be neglected, and general analytical results are available together with efficient numerical algorithms [1–3]. The situation is much more involved in the non-Markovian regime, which typically arises due to strong coupling and similar time scales of system and bath evolution. In this case general strategies are still available [2, 3], but differently from the Markovian case they typically lack simple results of general validity, to be expressed in terms of the phenomenologically relevant quantities and leading to manageable numerical tasks. A bridge between the two situations can be built relying on a suitable embedding of a non-Markovian dynamics in a Markovian one, as recently addressed in [4–6]. Indeed, while it is common wisdom that a non-Markovian process can be embedded in a Markovian one by a suitable enlargement of the number of relevant variables already at classical level [7], there is no universal recipe for how this can be done and which class of non-Markovian processes can be reached.

In the present Letter we demonstrate how such a Markovian reduction can be achieved for the ubiquitous model of quantum dissipation provided by a Brownian particle, or a two-level system, linearly coupled to a bath of harmonic oscillators characterized by an arbitrary spectral density (SD) [8]. The procedure is physically transparent, in that it focuses exclusively on the SD, and all relevant quantities can be constructed in terms of the SD. As will be shown below, the system dynamics can equivalently be described including, besides the Brownian particle degree of freedom, a set of effective environmental modes coupled in a linear-chain fashion. The terminal mode of the chain couples to a residual bath and undergoes a Brownian-like dynamics which rapidly approaches a Markovian behavior over the whole interval of relevant frequencies as the length of the chain increases. The model as such is closely related to Mori's theory [9] and its generalizations [10, 11]. While previous work by two of us [4, 5] has focused on the implications of a Markovian truncation of such effective mode chains, the present analysis proves the convergence towards Ohmic behavior, and thus the general validity of the procedure. The question of how to correctly set the initial state of the chain will be detailed in a forthcoming paper.

Effective-mode transformation. We start by considering the Caldeira-Leggett Hamiltonian, here written in mass-weighted bath coordinates x_k,

$$H = \frac{p^2}{2m} + V(s) + \frac{1}{2}\sum_{k=1}^{N}\left[p_k^2 + \omega_k^2\left(x_k - \frac{c_k}{\omega_k^2}s\right)^2\right] \quad (1)$$

which is known to lead, in the continuum limit, to a generalized Langevin dynamics for the system described by the s degree of freedom. The reduced system dynamics is entirely determined by the SD of the environmental coupling $J_0(\omega)$ which, for the microscopic model above,

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reads as [3]

$$J_0(\omega) = \frac{\pi}{2}\sum_{k=1}^{N}\frac{c_k^2}{\omega_k}\delta(\omega-\omega_k). \tag{2}$$

In general, $J_0(\omega)$ is a real, odd parity function defined by the real part of the frequency-dependent memory kernel [17] $\gamma(\omega)$ entering the generalized Langevin equation (GLE), namely $J_0(\omega) = m\omega \mathrm{Re}\gamma(\omega)$ and $J_0(\omega) \geqslant 0$ for $\omega > 0$. It fully determines $\gamma(\omega)$ by virtue of the Kramers-Kronig relations, as well as the correlation function of the GLE random force by virtue of the fluctuation-dissipation theorem. In the following we assume, as a typical situation, that $J_0(\omega)$ is strictly positive and continuous in an interval $(0, \omega_R)$ - where ω_R is a high-frequency cutoff - and zero otherwise on the positive real axis; other interesting cases will be briefly considered below.

Given a GLE and its relevant SD J_0, Eq.(2) allows to define a microscopic model for the dissipative dynamics of the s degree of freedom, *e.g.* by introducing a bath of harmonic oscillators with evenly spaced frequencies $\omega_k = k\Delta\omega$ $(k = 1, \ldots, N)$ and setting the coupling coefficients of Eq.(1) as

$$c_k = \sqrt{\frac{2\omega_k \Delta\omega J_0(\omega_k)}{\pi}} \tag{3}$$

The system-bath interaction term in Eq.(1), $H^{int} = -\sum_{k=1}^{N} c_k x_k s = -D_0 X_1 s$, naturally introduces an effective mode $X_1 = \sum_{k=1}^{N} c_k x_k / D_0$ where D_0 is a normalization constant which in the continuum limit reads $D_0^2 = \sum_{k=1}^{N} c_k^2 \approx \frac{2}{\pi}\int_0^\infty d\omega J_0(\omega)\omega$. This defines the first column of an otherwise arbitrary, orthogonal matrix $\boldsymbol{T}$ transforming the bath coordinates $\boldsymbol{x}^t = (x_1, \ldots, x_N)$ into $\boldsymbol{X}^t = (X_1, X_2', \ldots, X_N')$, $\boldsymbol{X} = \boldsymbol{T}^t\boldsymbol{x}$. The transformation can be fixed by requiring that the "residual" bath of coordinates $X_2', X_3', \ldots, X_N'$ is in normal form, *i.e.* that $(\boldsymbol{T}^t\boldsymbol{\omega^2}\boldsymbol{T})_{ij} = \delta_{ij}\bar{\Omega}_i^2$ holds for all $i, j > 1$ with $(\boldsymbol{\omega^2})_{ij} = \delta_{ij}\omega_i^2$ $(i, j = 1, \ldots, N)$. Note that the frequency Ω_1 of the effective mode introduced in this way is solely determined by the SD $J_0(\omega)$, $\Omega_1^2 = (\boldsymbol{T}^t\boldsymbol{\omega^2}\boldsymbol{T})_{11} = \sum_{k=1}^{N}\omega_k^2 c_k^2/D_0^2 \approx \frac{2}{\pi D_0^2}\int_0^\infty d\omega J_0(\omega)\omega^3$. The couplings $C_k = -(\boldsymbol{T}^t\boldsymbol{\omega^2}\boldsymbol{T})_{1,k}$ $(k = 2, \ldots, N)$ between the normal modes of the residual bath and X_1 allow one to re-write Eq.(1) as a Caldeira-Leggett-like Hamiltonian for the X_1 degree of freedom, thereby defining the SD $J_1(\omega) = \frac{\pi}{2}\sum_{k=2}^{N}\frac{C_k^2}{\bar{\Omega}_k}\delta(\omega - \bar{\Omega}_k)$ "felt" by the effective mode X_1, which is the only bath mode directly coupled to the s degree of freedom. Clearly, in the continuum limit, the procedure can be indefinitely iterated and used to define a sequence of effective modes $X_1, X_2, \ldots, X_M, \ldots$ coupled in a linear-chain fashion *and* a corresponding sequence of SD $J_1, J_2, \ldots, J_M, \ldots$ characterizing the residual bath "felt" by each mode, see Fig.1. In other words, there exists an orthogonal coordinate transformation which converts the continuum version of Eq.(1) into the form

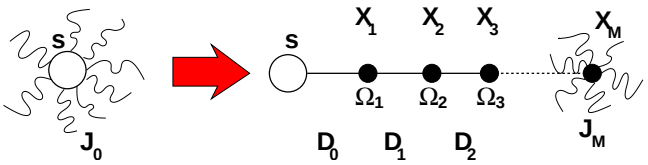

Figure 1: (Color online) Schematic for the linear-chain transformation described in the text. X_n are the effective modes, Ω_n their frequencies and D_n the couplings between adjacent modes X_{n-1} and X_n ($X_0 = s$). The SD J_M $(M \geq 0)$ describe the interaction with the residual bath.

$$\begin{aligned} H \quad &= \tfrac{p^2}{2m} + V(s) + \Delta V(s) - D_0 s X_1 + \\ &- \textstyle\sum_{n=1}^{\infty} D_n X_n X_{n+1} + \frac{1}{2}\sum_{n=1}^{\infty}\left[P_n^2 + \Omega_n^2 X_n^2\right] \end{aligned} \tag{4}$$

where, for $n \geqslant 0$,

$$D_n^2 = \frac{2}{\pi}\int_0^\infty d\omega J_n(\omega)\omega, \;\; \Omega_{n+1}^2 = \frac{2}{\pi D_n^2}\int_0^\infty d\omega J_n(\omega)\omega^3$$

$$X_{n+1} = \sqrt{\frac{2}{\pi D_n^2}}\int_0^\infty \omega\sqrt{J_n(\omega)}x(\omega)d\omega$$

(and similarly for P_{n+1} in terms of $p(\omega)$); $\Delta V(s) = \delta\Omega_0^2 s^2/2$ is a counter term involving the renormalization frequency $\delta\Omega_0^2 = (2/\pi)\int_0^\infty d\omega J_0(\omega)/\omega$. As we show below, though different canonical transformations to a linear chain be devised (see e.g. Ref. 12), the one suggested above, with the coupling in pure coordinate form, allows one to write an explicit expression for $\{J_n\}_{n\in\mathbb{N}}$ *without* knowing the eigenfrequencies of the residual bath at each step.

Sequence of SD. As observed by Leggett [13, 14], the SD acting on the system degree of freedom can be obtained from the analytically continued, Fourier-transformed classical (or Heisenberg) equations of motion as the imaginary part of a propagator,

$$J_0(\omega) = -\lim_{\epsilon\to 0^+}\mathrm{Im}L_0(\omega + i\epsilon) \equiv -\mathrm{Im}L_0^+(\omega).$$

This procedure has recently been used by two of us to obtain a continued-fraction expression for the SD generated by a linear chain with Markovian closure, which in turn formed the basis for approximating a given SD [4, 5]. Employing a similar strategy, we now focus on the properties of the residual spectral densities J_M closing the chain after M effective modes have been extracted as outlined above. For the Hamiltonian of Eq.(1), after introducing the first effective mode X_1, we obtain

$$L_0(z) = -z^2 - \cfrac{D_0^2}{\Omega_1^2 - z^2 - \sum_k \cfrac{C_k^2}{\bar{\Omega}_k^2 - z^2}}$$

where $\bar{\Omega}_k$ and C_k have been introduced above. In the continuum limit, with the help of Eq.(3), the sum in the denominator can be replaced by the function [18]

$$W_1(z) = \sum_{k=2}^{N} \frac{C_k^2}{\bar{\Omega}_k^2 - z^2} \approx \frac{2}{\pi} \int_0^\infty d\omega \frac{J_1(\omega)\omega}{\omega^2 - z^2}$$

or, equivalently,

$$W_1(z) = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{J_1(\omega)}{\omega - z}. \tag{5}$$

In this form W_1 is given as an integral of its limiting imaginary part, $J_1(\omega) = \mathrm{Im} W_1^+(\omega)$. In the following, a function W_1 defined by Eq.(5) will be referred to as the *Cauchy transform* of J_1 [15]; it is an analytic function in the whole complex plane except for the support of J_1 on the real axis [19], which vanishes as z^{-2} for $|z| \to \infty$. We *define*

$$W_0(z) = \frac{D_0^2}{\Omega_1^2 - z^2 - W_1(z)} \tag{6}$$

which, analogously to $L_0 = -z^2 - W_0$, gives $J_0(\omega) = \mathrm{Im} W_0^+(\omega)$. It follows that J_1 can be written in terms of J_0 as $J_1(\omega) = \frac{D_0^2 J_0(\omega)}{|W_0^+(\omega)|^2}$ where, as we now show, W_0 is the Cauchy transform of J_0. In order to prove this, we notice that according to its definition, Eq.(6), W_0 is analytic in the upper and lower half planes [20], and vanishes as z^{-2} for $|z| \to \infty$. Writing $W_0(z)$ as a Cauchy integral on a large semicircle in the upper half plane, we can add a term $\pm(\omega - z^*)^{-1}$ to the integrand, and get, from the real and imaginary parts of the resulting expression, the desired result. In general, then

$$J_{n+1}(\omega) = \frac{D_n^2 J_n(\omega)}{|W_n^+(\omega)|^2} \tag{7}$$

defines a recurrence relation for the SD $J_{n+1}(\omega)$ felt by the $n+1$-th effective mode, given the SD $J_n(\omega)$ of the n-th mode. Equivalently[21],

$$W_{n+1}(z) = \Omega_{n+1}^2 - z^2 - \frac{D_n^2}{W_n(z)} \tag{8}$$

is a recurrence relation for the Cauchy transforms which only requires the first Cauchy transform (W_0) as an input and easily provides the sequence $J_n(\omega) = \mathrm{Im} W_n^+(\omega)$.

Eq.(8) represents the main result of this Letter. It is a simple recurrence relation between the Cauchy transforms of the SDs which allows us to write the limiting condition as

$$W(z) = \Omega^2 - z^2 - \frac{D^2}{W(z)}$$

provided $\Omega = \lim_n \Omega_n$ and $D = \lim_n D_n$ exist. The physical solution ($\mathrm{Im} W^+ \geqslant 0$) provides the SD "closing"

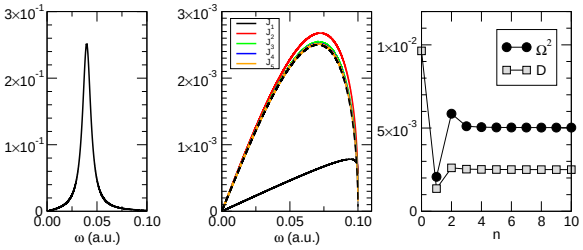

Figure 2: (Color online) Left: the SD J_0 defined in Eq.(11) for $\omega_0 = 0.04$ a.u., $d_0 = 0.01$ a.u. and $\gamma = 0.01$ a.u.. Middle: results of the deconvolution of J_0 for the first five modes, obtained when setting the high-frequency cutoff ω_R to 0.1 a.u.. The Rubin SD of Eq.(10) with the same ω_R is shown as dashed line. Right: Effective modes parameters (Ω_n^2 and D_n) up to $n = 10$.

the chain, which has a non-vanishing value for $\omega^2 \in [\Omega^2 - 2D, \Omega^2 + 2D]$ only. In other words, the limiting SD reads as

$$J(\omega) = \frac{1}{2}\sqrt{(\omega^2 - \omega_L^2)(\omega_R^2 - \omega^2)} \quad \omega_L \leq \omega \leq \omega_R \tag{9}$$

where $\omega_R^2 = \Omega^2 + 2D$ and $\omega_L^2 = Max\{\Omega^2 - 2D, 0\}$. The requirement $J_0(\omega) > 0$ for $\omega > 0$ fixes $\Omega^2 = 2D$, since the condition $\Omega^2 > 2D$ (though physically admissible) would give rise (using the above recursion procedure backwards) to a SD J_0 with a low-frequency cutoff $\omega_L = \sqrt{\Omega^2 - 2D}$. Therefore [22], $\Omega^2 = 2D$, $\omega_R^2 = 4D = 2\Omega^2$ and Eq.(9) reduces to the quasi-Ohmic SD provided by the Rubin model of dissipation [3, 16],

$$J_{Rubin}(\omega) = \frac{\omega\omega_R}{2}\sqrt{1 - \frac{\omega^2}{\omega_R^2}}\Theta(\omega_R - \omega). \tag{10}$$

This means that provided a sufficient number of effective modes is included in the definition of the system, the resulting dynamics is Markovian. In practice, as we show numerically below this number is rather small, since convergence is quite fast even for structured spectral densities. Notice though that when $J_0(\omega)$ has a low frequency cutoff ω_L but is otherwise positive on the interval (ω_L, ω_R), Eq.(9) shows that no Markovian reduction is possible, no matter how many effective modes are included in the system.

In general, a high-frequency cutoff ω_R can be naturally associated to the SD $J_0(\omega)$, determining the spectrum of environmental frequencies relevant for the reduced system's dynamics. This suffices to show that $\mathrm{Re} W_0^+(\omega)$ diverges logarithmically for $\omega \to \omega_R$, unless $J_0(\omega_R)$ is equal to zero. In view of Eq.(7) this in turn implies that $J_1(\omega) \to 0$ as $\omega \to \omega_R$, and this cutoff is later on automatically preserved. Furthermore, starting from Eq.(8) one can also immediately obtain some interesting bounds on the value $\mathrm{Re} W_n^+(\omega)$ can take at the extreme points of the relevant frequency interval $(0, \omega_R)$, which help determine the behavior of the recurrence relation

Eq.(7). Among these we only note here that $\mathrm{Re}W_n^+(\omega)$ is positive for $\omega = 0$ and negative for $\omega = \omega_R$, and then by continuity the function will go through zero at some intermediate point $\bar{\omega}$. This explains why the procedure generally fails to converge for SD with gaps, since if $\bar{\omega}$ falls in the gap one has $W_n^+(\bar{\omega}) = 0$ and, by virtue of Eq.(8), this introduces an isolated pole in $W_{n+1}(z)$ which invalidates the use of Eq.(5). Notice, however, that even in this case an orthogonal transformation of bath variables into linear-chain modes can still be introduced to define a number of chains of effective modes, one for each interval where $J_0(\omega) > 0$.

Numerical results. The procedure described above for the determination of the sequence $\{J_n\}_{n\in\mathbb{N}}$ of effective SD can be easily implemented numerically, relying on the recurrence relation Eq.(8) for the SD Cauchy transforms[23], the only necessary input being the initial SD J_0 and the cutoff ω_R. To show the effectiveness of the method and rapidity of convergence we consider the numerical results for a couple of representative SDs, with a frequency cutoff ω_R fixed in such a way that $J_0(\omega_R) \approx 0$. As a first example we consider

$$J_0(\omega) = \frac{d_0^2\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}, \qquad (11)$$

which is the effective SD felt by a Brownian particle coupled to a harmonic oscillator of frequency ω_0 which in turn interacts with an Ohmic bath[14]. This coupling scheme is evident from the results of Fig.2 where J_1, plotted in the middle panel, appears to be Ohmic, as can also be checked analytically. The sequence then very rapidly becomes indistinguishable from the Rubin SD given by Eq.(10) for the chosen cutoff ω_R, as can also be seen from the ratio $\Omega_n^2/D_n \to 2$. As a second example we consider a highly structured, multipeaked SD as plotted in Fig.3. It is clear from the figure that also in this case convergence is quite fast, and the limiting Rubin SD is obtained after few (say 10-15) iterations.

Conclusions. We have presented a recursive procedure to recast the non-Markovian dynamics of a Brownian particle, interacting with a bath characterized by an arbitrary SD, into the Markovian dynamics of an enlarged set of variables including effective modes of the reservoir coupled to a quasi-Ohmic residual SD. The approach provides an explicit analytic relationship among successive residual SD, which can be easily evaluated numerically starting from an arbitrary (gapless) initial SD. These results pave the way for an efficient general treatment of quantum dissipation in the presence of arbitrarily complex environments.

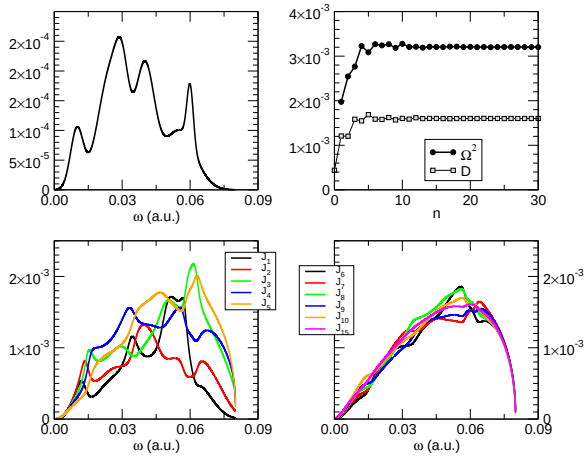

Figure 3: (Color online) Deconvolution of the highly structured SD J_0 shown in the upper left panel, with $\omega_R = 0.08$ a.u.. Top right: effective mode parameters up to $n = 30$. Bottom: the sequence J_n for $n = 1, \ldots, 15$.

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[17] Here and in the following we define the Fourier transform as $\gamma(\omega) = \int_{-\infty}^{+\infty} \gamma(t)e^{i\omega t}dt$.

[18] This is legitimate since the (unknown) eigenfrequencies $\bar{\Omega}_k$ satisfy $\omega_1 \leq \bar{\Omega}_2 \leq \omega_2 ... \leq \bar{\Omega}_N \leq \omega_N$, thereby covering uniformly the interval $(0, \omega_R)$ as $\Delta\omega \to 0$.

[19] In the presence of a cutoff ω_R the upper and lower half planes are connected through the semiaxes $|\omega| > \omega_R$. Note also that we consider only Cauchy transforms of odd functions.

[20] The denominator vanishes on the real axis only, since $\Omega_1^2 - z^2 - W_1(z) = 0$ is the eigenvalue equation defining the frequencies ω_k appearing in Eq.(1).

[21] According to Eq.(7) the Cauchy transform of J_{n+1} must

be of the form $W_{n+1}(z) = g_{n+1}(z) - \frac{D_n^2}{W_n(z)}$ where $g_{n+1}(z)$ is an analytic function with vanishing imaginary part on the real axis, uniquely fixed by asking that it offsets the behavior of $W_n^{-1}(z)$ as $|z| \to \infty$, $W_n(z) \approx -\frac{D_n^2}{z^2}\left(1 + \frac{\Omega_{n+1}^2}{z^2} + ...\right)$.

[22] When $\Omega^2 \leq 2D$, D and Ω are functions of ω_R only (see Eq.(9)). It follows, from their definition, $\Omega^2 = 2D$.

[23] Results are numerically indistinguishable from those obtained by applying the recursion of Eq.(7) or by computing the eigenfrequencies of the residual bath discretized at each step.